First- and second-order superfluid–Mott-insulator phase transitions of spin-1 bosons with coupled ground states in optical lattices

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We investigate the superfluid–Mott-insulator quantum phase transition of spin-1 bosons in an optical lattice created by pairs of counterpropagating linearly polarized laser beams, driving an $F_g = 1$ to $F_e = 1$ internal atomic transition. The whole parameter space of the resulting two-component Bose-Hubbard model is studied. We find that the phase transition is not always second order as in the case of spinless bosons, but can be first order in certain regions of the parameter space. The calculations are done in the mean-field approximation by means of exact numerical diagonalization as well as within the framework of perturbaton theory.

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The superfluid–Mott-insulator quantum phase transition (SMQPT) of spinless bosons in periodic lattices is a second-order transion, which is characterized by a continuous variation of the order parameter ψ from $\psi \neq 0$ (superfluid phase) to $\psi = 0$ (Mott-insulator phase) if the amplitude of the lattice potential increases [1, 2]. In our recent paper [3], we have shown that the SMQPT in a system of spin-1 bosons can be first order as well [4]. By means of numerical calculations within the framework of the mean-field theory, it was found that in the case of ^{23}Na the SMQPT is second order if the number of atoms per lattice site $n = 1, 3$, and it is first order for $n = 2$. In the case of ^{87}Rb, the SMQPT was found to be second order for $n = 1, 2, 3$. In the present work, we continue the study of Ref. [3]. The main purpose is to investigate the whole parameter space of spin-1 bosons and to find the regions where the SMQPT is first and second order for arbitrary n.

We consider spin-1 neutral polarizable bosons, possessing three Zeeman-degenerate internal ground and excited electronic states characterized by the magnetic quantum number $m = 0, \pm 1$ ($F_g = F_e = 1$) in a d-dimensional ($d = 1, 2, 3$) optical lattice. The lattice is assumed to be created by d pairs of counterpropagating linearly polarized laser waves running in d orthogonal directions and having different frequencies in different directions. The beams propagating along the 3-axis, which is chosen to be a quantization axis, are polarized along the 1- or 2-axis, and the beams propagating along the 1- and 2-axis are polarized along the 2- and 1-axis, respectively.

The running laser waves form left- and right-polarized standing waves with Rabi frequencies $\Omega_\nu(r_\nu) = \Omega_{0\nu}\cos(k_L r_\nu)$, which couple internal ground and excited states by V- and Λ- transitions. In order to avoid decoherence due to spontaneous emission, the detunings Δ_i must satisfy the conditions $|\Delta_\nu| \gg \gamma$, where γ is the spontaneous emission rate. If the laser intensities and the detunings are chosen in such a manner that $\Omega_{0\nu}^2/\Delta_\nu = \Omega_0^2/\Delta$, $\nu = 1, \ldots, d$, the laser potential acting on the atomic ground states is given by the matrix

$$V_L(\mathbf{r}) = \hbar\frac{\Omega_0^2}{\Delta}\sum_{\nu=1}^{d}\cos^2(k_L r_\nu)\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad (1)$$

which determines the isotropic lattice potential with the period π/k_L and at the same time couples the atomic ground states with $m = \pm 1$. In the case of red detuning $\Delta < 0$, the system is described by the two-component Bose-Hubbard Hamiltonian [3]

$$\begin{aligned}\hat{H}_{BH} = &-J\sum_{<i,j>}\left(\hat{a}_{0i}^\dagger\hat{a}_{0j} + \hat{a}_{\Lambda i}^\dagger\hat{a}_{\Lambda j}\right) \\ &+\sum_i\left[\frac{U_s}{2}\hat{n}_i(\hat{n}_i - 1) + U_a\hat{n}_{0i}\hat{n}_{\Lambda i}\right. \\ &\left.-\frac{|U_a|}{2}\left(\hat{a}_{0i}^\dagger\hat{a}_{0i}^\dagger\hat{a}_{\Lambda i}\hat{a}_{\Lambda i} + \hat{a}_{\Lambda i}^\dagger\hat{a}_{\Lambda i}^\dagger\hat{a}_{0i}\hat{a}_{0i}\right) - \mu\hat{n}_i\right], \qquad (2)\end{aligned}$$

where μ is a chemical potential and the operator $\hat{n}_i = \hat{n}_{0i} + \hat{n}_{\Lambda i}$. The indices i, j label the lattice sites, and $\hat{a}_{\sigma i}$ is the Bose annihilation operator for the component $\sigma = 0, \Lambda$ attached to the ith lattice site. The tunneling matrix element

$$J = -\int W_{i+1}(\mathbf{r})\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\mathbf{r}^2} + V_{L0}(\mathbf{r})\right]W_i(\mathbf{r})\,d\mathbf{r},$$

where $W_i(\mathbf{r})$ is the Wannier function for the lowest Bloch band of the potential

$$V_{L0}(\mathbf{r}) = 2\hbar\frac{\Omega_0^2}{\Delta}\sum_{\nu=1}^{d}\cos^2(k_L r_\nu),$$

is a rapidly varying function of the laser intensity [6]. The variations of the atomic interaction parameters

$$U_{s,a} = g_{s,a}\int W_i^4(\mathbf{r})\,d\mathbf{r}$$

are much slower [6]. The quantities $g_{s,a}$ describe the repulsive interaction of the condensate atoms and the spin-changing collisions. The parameter U_s is positive, but U_a can be either positive or negative depending on the sign of g_a.

In order to investigate the SMQPT, we employ the mean-field approximation [1, 2]

$$\hat{a}_{\sigma i}^\dagger\hat{a}_{\sigma j} \approx \psi_\sigma\left(\hat{a}_{\sigma j} + \hat{a}_{\sigma i}^\dagger\right) - \psi_\sigma^2, \qquad (3)$$

where ψ_σ is the order parameter for Bose-Einstein condensation in the component $\sigma = 0, \Lambda$, which can be considered

as a real quantity. In this approximation, the Bose-Hubbard Hamiltonian becomes local and every lattice site is described by the Hamiltonian

$$\begin{aligned}\hat{H}'_{BH} &= \hat{H}^{(0)} + \hat{V} \,, \\ \hat{H}^{(0)} &= 2dJ\left(\psi_0^2+\psi_\Lambda^2\right) + \frac{U_s}{2}\hat{n}(\hat{n}-1) \\ &\quad + U_a\left[2\hat{T}^2_{1(2)} - \frac{\hat{n}}{2}\right] - \mu\hat{n} \,, \\ \hat{V} &= -2dJ\left[\left(\hat{a}_0^\dagger + \hat{a}_0\right)\psi_0 + \left(\hat{a}_\Lambda^\dagger + \hat{a}_\Lambda\right)\psi_\Lambda\right] \,,\end{aligned} \tag{4}$$

where the index $1(2)$ corresponds to $U_a < 0$ ($U_a > 0$). In Eq.(4), we have omitted the site index i and introduced the isospin operator $\hat{\mathbf{T}}$ with the components

$$\begin{aligned}\hat{T}_1 &= \left(\hat{a}_\Lambda^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_\Lambda\right)/2 \,, \\ \hat{T}_2 &= i\left(\hat{a}_\Lambda^\dagger \hat{a}_0 - \hat{a}_0^\dagger \hat{a}_\Lambda\right)/2 \,, \\ \hat{T}_3 &= \left(\hat{a}_0^\dagger \hat{a}_0 - \hat{a}_\Lambda^\dagger \hat{a}_\Lambda\right)/2 \,,\end{aligned} \tag{5}$$

which has the property

$$\hat{\mathbf{T}}^2 = \frac{\hat{n}}{2}\left(\frac{\hat{n}}{2}+1\right) \,.$$

If the tunneling $\hat{V}$ is negligible, the eigenstates of the Hamiltonian (4) are determined by $H^{(0)}$ and can be calculated analytically. They are eigenstates $|n/2,\mathcal{M}\rangle$ of the isospin operator with the corresponding eigenenergies given by

$$\begin{aligned}E^{(0)}_{n/2,\mathcal{M}} &= 2dJ\left(\psi_0^2+\psi_\Lambda^2\right) + \frac{U_s}{2}n(n-1) \\ &\quad + U_a\left(2\mathcal{M}^2 - \frac{n}{2}\right) - \mu n \,,\end{aligned} \tag{6}$$

where n is the number of atoms per lattice site and $\mathcal{M} = -n/2,\ldots,n/2$ is the isospin projection on the direction $1(2)$ in the isospin space for the case of $U_a < 0$ ($U_a > 0$). Note that $n/2$ plays the role of the isospin quantum number. If n is even, the states with $\mathcal{M} = 0$ are not degenerate, while the others with $\mathcal{M} \neq 0$ are doubly degenerate. If n is odd, the states with $\mathcal{M} = 0$ do not exist and, therefore, all the eigenstates of $\hat{H}^{(0)}$ are doubly degenerate. If $U_a < 0$, the ground-state energy $E_g(\psi_0,\psi_\Lambda) = E^{(0)}_{n/2,\pm n/2}$, and the chemical potential μ varies in the interval

$$n-1 < \frac{\mu}{U_s - |U_a|} < n \,, \quad n = 1,2,\ldots$$

In the case of $U_a > 0$, $E_g(\psi_0,\psi_\Lambda) = E^{(0)}_{n/2,\pm 1/2}$ and

$$U_s(n-1) < \mu < U_s n - U_a \,,$$

if n is odd. If $U_a > 0$ and n is even, $E_g(\psi_0,\psi_\Lambda) = E^{(0)}_{n/2,0}$ and

$$U_s(n-1) - U_a < \mu < U_s n \,.$$

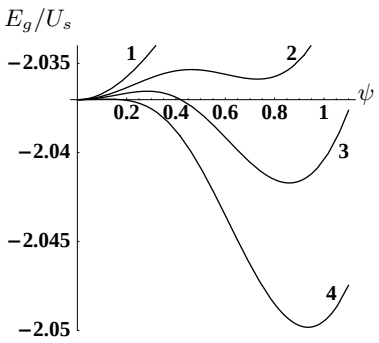

FIG. 1: Ground-state energy of the Hamiltonian (4) for ^{23}Na ($U_a/U_s \approx 0.037$ [7]). $\mu/U_s = 1.5$, $2dJ/U_s = 0.125(1), 0.148(2), 0.157(3), 0.167(4)$.

The minimum of E_g in all the cases is reached at $\psi_0 = \psi_\Lambda = 0$ and the system has a vanishing compressibility; i.e., it is in the Mott-insulator phase. Since $\langle n/2,\mathcal{M}|\hat{T}_3|n/2,\mathcal{M}\rangle = 0$, if $\mathcal{M}$ is the isospin projection on the direction 1 or 2, the mean occupation numbers of the componets $\langle n/2,\mathcal{M}|\hat{n}_0|n/2,\mathcal{M}\rangle = \langle n/2,\mathcal{M}|\hat{n}_\Lambda|n/2,\mathcal{M}\rangle = n/2$.

In order to investigate the transition from the Mott phase into the superfluid phase, one has to calculate the ground-state energy of the complete Hamiltonian (4). This can be done exactly by numerical calculations or approximately treating the tunneling $\hat{V}$ as a perturbation. Let us consider the case $U_a < 0$ first. Nonvanishing matrix elements of the operator $\hat{V}$ are given by

$$\begin{aligned}\left\langle \frac{n-1}{2},\mathcal{M}\mp\frac{1}{2}\middle|\hat{V}\middle|\frac{n}{2},\mathcal{M}\right\rangle &= -dJ\sqrt{n\pm 2\mathcal{M}} \\ &\quad\times\ (\psi_\Lambda \pm \psi_0)\exp\left(\mp i\pi/4\right),\end{aligned} \tag{7}$$

which implies that the ground-state energy E_g is independent of the sign of ψ_σ, $E_g(\psi_\Lambda,\psi_0) = E_g(|\psi_\Lambda|,|\psi_0|)$, and it is a symmetric function of ψ_0 and ψ_Λ: $E_g(\psi_0,\psi_\Lambda) = E_g(\psi_\Lambda,\psi_0)$. The minima of E_g are located on the lines $\psi_\Lambda = \pm\psi_0$ [3]. Therefore, for the calculation of the phase diagram of the system one can set $\psi_\Lambda = \pm\psi_0 \equiv \psi$. Employing the perturbation theory we found that E_g has the structure

$$E_g(\psi) = a_0 + a_2\psi^2 + a_4\psi^4 + \ldots \,, \tag{8}$$

where a_2 can be either positive or negative, but a_4 is always positive, which means that the SMQPT is second order. The boundary between the Mott and superfluid phases is determined from the condition $a_2 = 0$ and given by

$$\tilde{J} = (1-n+\tilde{\mu})(n-\tilde{\mu})/(1+\tilde{\mu}) \,, \tag{9}$$

where $\tilde{J} = 2dJ/(U_s - |U_a|)$ and $\tilde{\mu} = \mu/(U_s - |U_a|)$, similar to the case of spinless bosons [1, 2]. This equation agrees perfectly with the results obtained by numerical diagonalization.

In the case of positive U_a, the situation is quite different.

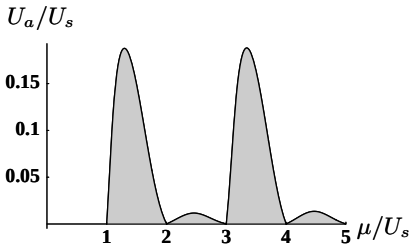

FIG. 2: In the shaded regions of this diagram, a_4 is negative and $E_g(\psi)$ has two minima at certain values of J. In the remaining part a_4 is positive and $E_g(\psi)$ has only one minimum.

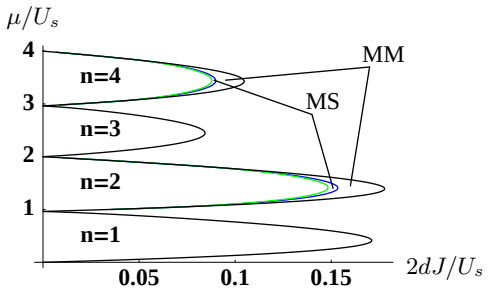

FIG. 3: Phase diagram for ^{23}Na ($U_a/U_s \approx 0.037$ [7]). The regions of metastable superfluid phase coexisting with the stable Mott phase and that of metastable Mott phase coexisting with the stable superfluid phase are denoted by MS and MM, respectively.

Since the matrix elements of the operator $\hat{V}$ are given by

$$\left\langle \frac{n-1}{2}, \mathcal{M} \mp \frac{1}{2} \middle| \hat{V} \middle| \frac{n}{2}, \mathcal{M} \right\rangle = -dJ\sqrt{n \pm 2\mathcal{M}} \times \left(\psi_0 e^{i\pi/4} \mp \psi_\Lambda e^{-i\pi/4} \right) , \quad (10)$$

the ground-state energy E_g depends only on $\psi^2 = \psi_0^2 + \psi_\Lambda^2$. Typical dependences $E_g(\psi)$ obtained by numerical diagonalization are shown in Fig. 1. In contrast to the case of negative U_a, there can be one or two minima. This leads to the fact that the QPT can be not only first order but also second order and the superfluid and Mott phases can coexist in certain parts of the phase diagram. Analytical calculations within the framework of the perturbation theory show that E_g has the form (8), but now not only a_2 but also a_4 can be either positive or negative. Therefore, in order to be able to work out the complete phase diagram analytically, one has to calculate a_6 in Eq.(8). This is a tedious task and we have not done that. However, solving the equation $a_4(\mu/U_s, U_a/U_s) = 0$ one can determine the regions in the plane $(\mu/U_s, U_a/U_s)$, where E_g can have one and two minima; i.e., one can find the regions where the SMQPT is second and first order, respectively. These regions, which are shown in Fig. 2, can be also found by numerical diagonalization and the result appears to be the same. Our analytical as well as numerical calculations show that, for $n = 1$, $E_g(\psi)$ has only one minimum and the SMQPT is always second order. If $n \geq 2$, $E_g(\psi)$ can have either one or two minima, depending on the parameters, and the SMQPT can be either second or first order. If, at a fixed n, U_a/U_s is larger than some critical value, which is about 0.188 for even n and grows from 0.012 ($n = 3$) to 0.015 ($n \to \infty$) for odd n, the QPT is second order; otherwise, it is first order. In the case of ^{23}Na shown in Fig. 3, an interesting regime is achieved, when the QPT for odd n is second order, but for even n it is first order.

The phase diagram for ^{23}Na presented in Fig. 3 has been obtained by numerical diagonalization. It consists of a series of (internal) lobes corresponding to the stable Mott phase and external regions corresponding to the stable superfluid phase. However, in the case of even n, the two regions are separated from one another by intermediate ones, where the stable and metastable superfluid and Mott phases coexist. The boundary separating the region of the stable superfluid phase from other ones can be determined from the condition $a_2 = 0$. If n is odd, it is given by

$$J' = 4\left[\frac{n-1}{\mu' - n + 1 + 2U_a'} + \frac{n+3}{n + U_a' - \mu'} + 2(n+1)\left(\frac{1}{n - U_a' - \mu'} + \frac{1}{\mu' - n + 1}\right)\right]^{-1} , \quad (11)$$

where $J' = 2dJ/U_s$, $U_a' = U_a/U_s$, and $\mu' = \mu/U_s$. For even n, the boundary is given by the equation

$$J' = \frac{(\mu' - n + 1 + U_a')(n - \mu')}{\mu' - n + 1 + U_a' + (1 + U_a')\, n/2} . \quad (12)$$

These analytical expressions describe perfectly the corresponding numerical results.

In conclusion, we have shown that in the laser configuration we consider, the SMQPT of spin-1 bosons with the ferromagnetic interactions ($U_a < 0$) is always second order and the boundary between the superfluid and Mott-insulator phases is given by Eq.(9). In the case of antiferromagnetic interactions, the SMQPT is first order in the shaded region of the plane (μ, U_a), shown in Fig. 2, and it is second order in the rest part of the plane.

Acknowledgments

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